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Hierarchical multilevel methods for exascale UQ and optimization

Challenges and Possible paths forward

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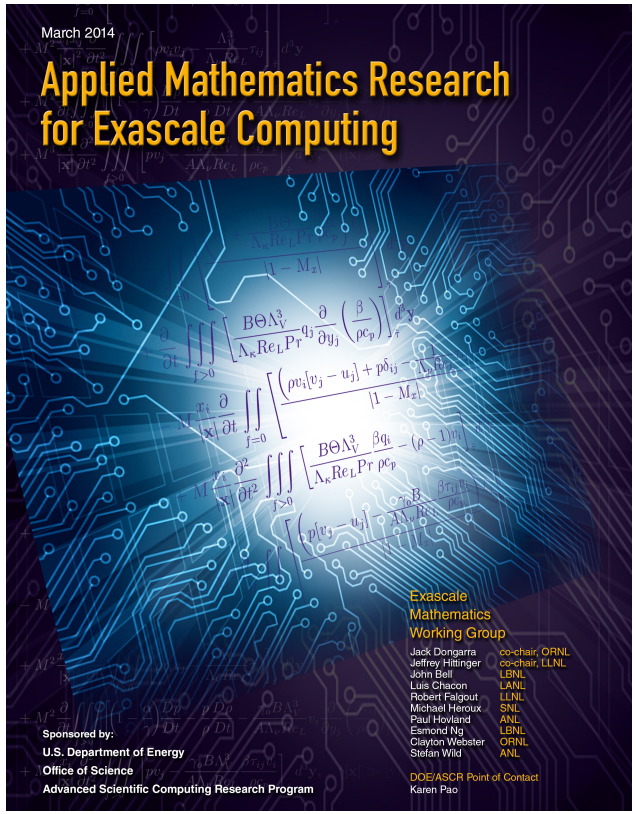
Outline

- See Section 4.2.2 and 4.2.3 in the *Applied Mathematics Research for Exascale* →



From petascale to exascale

Some challenges remain but new challenges (and opportunities) emerge

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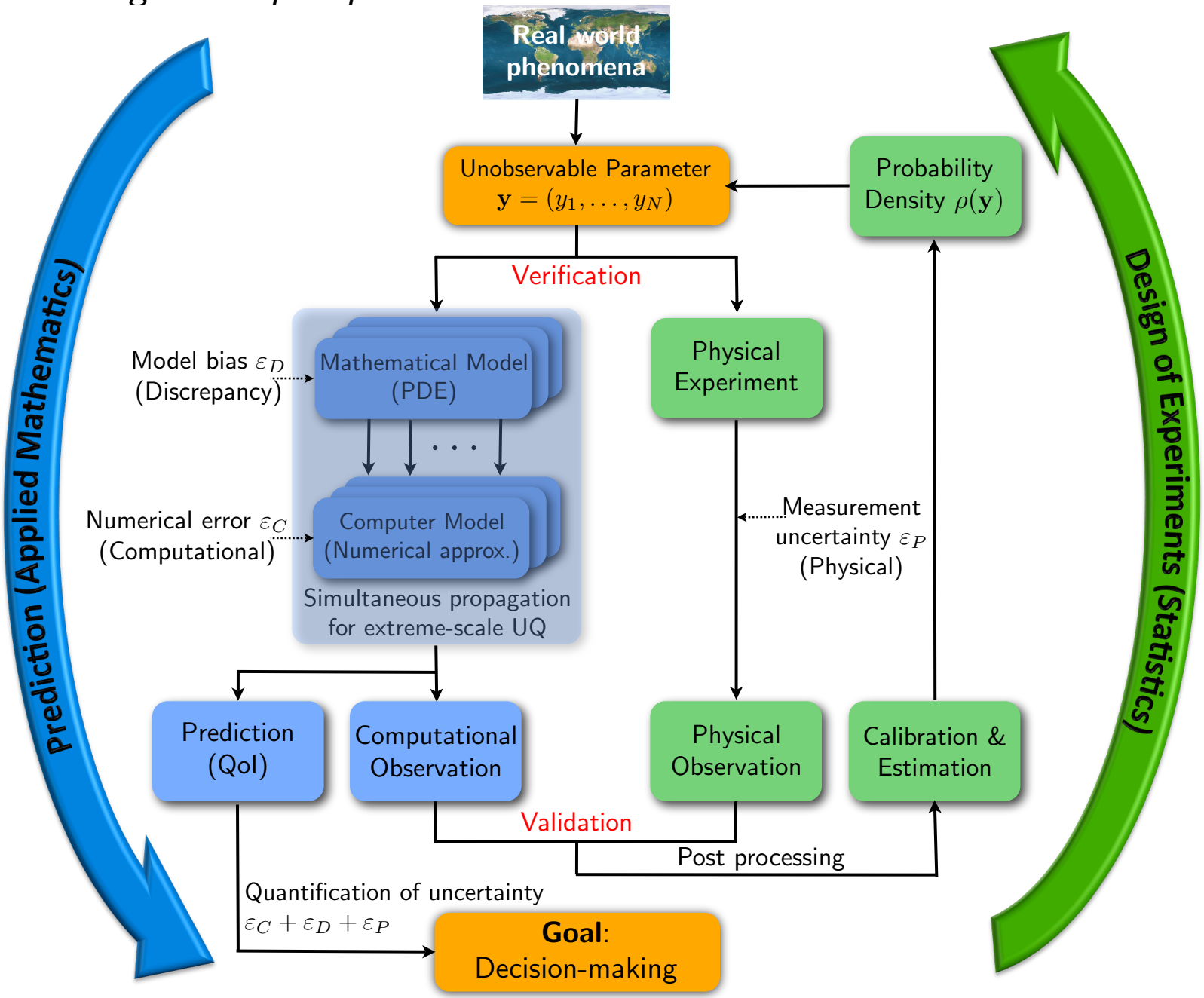
In moving towards exascale, several challenges arise when applying UQ methodologies to the DOE mission science areas.

1. Detection and quantification of high-dimensional stochastic QoIs with a specified certainty
2. Reducing the computational burden required to perform rigorous UQ
3. Efficient strategies for UQ that exploit greater levels of parallelism provided by emerging many-core architectures
4. Systematic assimilation of the uncertainty in measured data for validating and correcting model bias, calibrating parameter interrelations, and improving confidence in predicted responses

EQUINOX: *An architecture-aware, predictive capability for explaining how the uncertainties, ubiquitous in all modeling efforts affect our predictions and understanding of complex phenomena*



Forward UQ: PDEs with random input data

Complexity reduction for uncertainty quantification

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parameters $\boldsymbol{y}(\omega)$, $\omega \in \Omega_{\mathbb{P}}$ $\longrightarrow$ **SPDE model:** $\mathcal{L}(u, \boldsymbol{y}) = f$ for a.e. $x \in D \subset \mathbb{R}^d$ $\longrightarrow$ quantity of interest $Q[u(\cdot, \boldsymbol{y})]$

- The parameters $\boldsymbol{y}(\omega)$ may be affected by uncertainty (experimental data, incomplete description of parameters, unresolved scales, etc.)
- $\boldsymbol{y} : \Omega \to \Gamma \subset \mathbb{R}^N$ can be assumed to be a random vector with N components, i.e., $\boldsymbol{y} = (y_1, \ldots, y_N)$, with joint probability density function $\rho(\boldsymbol{y})$

The solution u is a stochastic function, $u(\cdot, \boldsymbol{y})$

Goals of forward UQ: Approximate u or some statistical QoI depending on u, i.e.

$$\mathbb{E}[u],\ \mathbb{V}\mathrm{ar}[u],\ \mathbb{P}[u > u_0] = \mathbb{E}[\mathbb{1}_{\{u>u_0\}}]$$

with as minimal computational cost as possible

Brief taxonomy of (current) numerical strategies

Stochastic FEMs [Gunzburger-W-Zhang, Acta Numerica 2014]

- Let $\mathcal{H}_M(\Gamma) = \{\boldsymbol{y}_m \in \Gamma\}_{m=1}^M$ denote a set of (possible random) sample points
- Let $u_h(x, \boldsymbol{y}_m) := u_h(\boldsymbol{y}_m)$ for $m = 1, \ldots, M$ denote the finite element approximation to the parametric PDE on a fixed mesh h

Monte Carlo methods

$$\mathbb{E}[u] \approx E_M[u_h] = \frac{1}{M} \sum_{m=1}^{M} u_h(x, \boldsymbol{y}_m)$$

pro: convergence rate is independent of N

con: asymptotic rate is $\mathcal{O}(1/\sqrt{M})$

Stochastic polynomial methods

- Stochastic Galerkin: projection technique, intrusive approach
- Stochastic collocation: interpolation technique, non-intrusive approach

$$u \approx u_{M,h}^{(SL)} = \sum_{m=1}^{M} c_m(x)\psi_m(\boldsymbol{y})$$

pro: convergence can be faster than MC

con: curse of dimensionality

- $\{\psi_m\} \in \mathcal{P}(\Gamma)$ polynomial basis and c_m determined through, e.g., $u_h(\boldsymbol{y}_m)$

Scalability constraints of current UQ

Näive implementations yield suboptimal efficiency

Exascale will require
... billion-way parallelism
... with less memory per core
... at potentially lower clock speeds

Current UQ approaches (both non-intrusive and intrusive) provide massive parallelism, but they don't scale (well) now and **won't** scale in the future:

- Independent simulation $\rightarrow$ easy parallelism...
  ... but independent instantiations $\rightarrow$ poor memory resource usage.
  This approach eats memory as fast as it fills compute cores

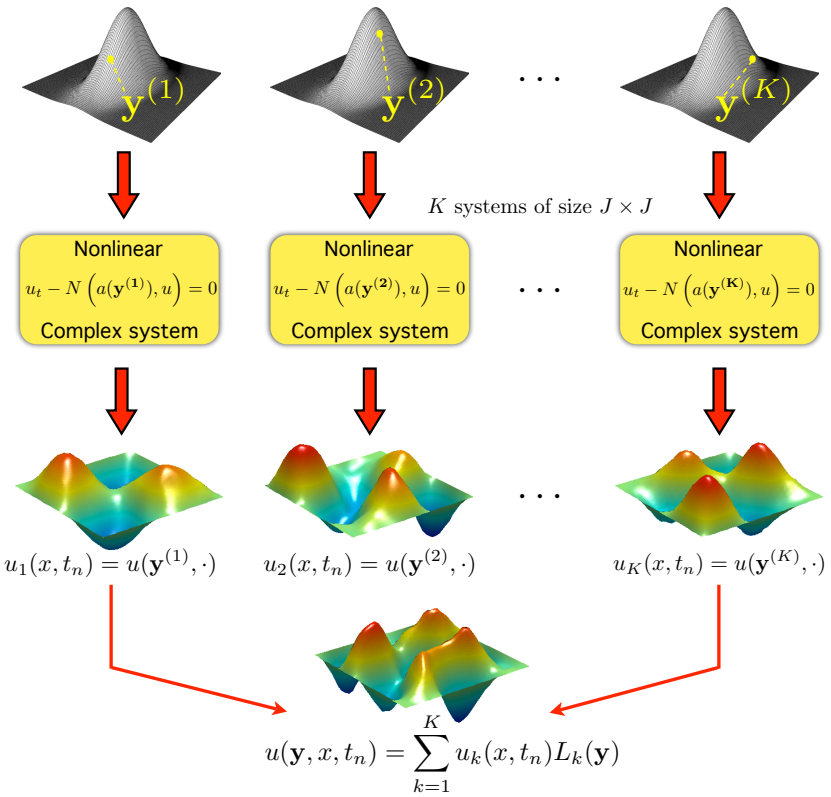
- Independent solves means that similarity between systems cannot be exploited for improved efficiency

- Process-level parallelism is simple, but finer-grained parallelism (thread and vector) is superior

This näive approach is ultimately too restrictive

An embedded UQ paradigm

Simultaneous propagation on ensembles



Key Idea: Simultaneous propagation of samples through a single program instantiation, allowing:

- block solvers to exploit related systems to accelerate solver convergence
- finer-grained parallelism to yield speedup even for a single core
- shared-memory parallelism to permit sharing common data and reducing contention for memory resources

Result: faster time-to-solution, independent of parallel speedup (esp. important if power/reliability require slower clock speeds) and reduced memory resources

These benefits are significant on current architectures, and will be crucial for future extreme-scale architectures

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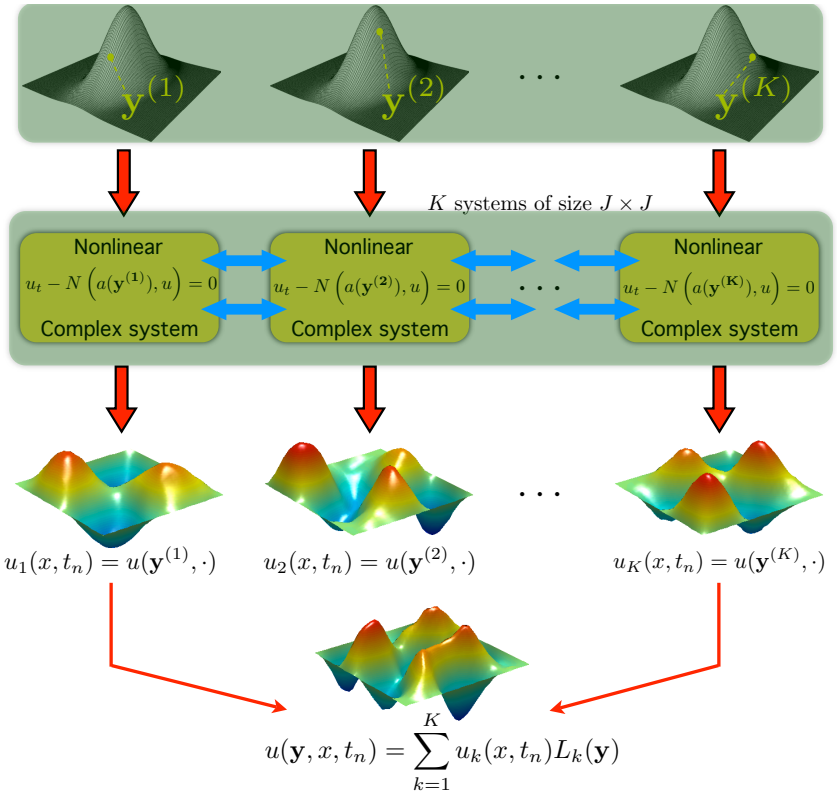

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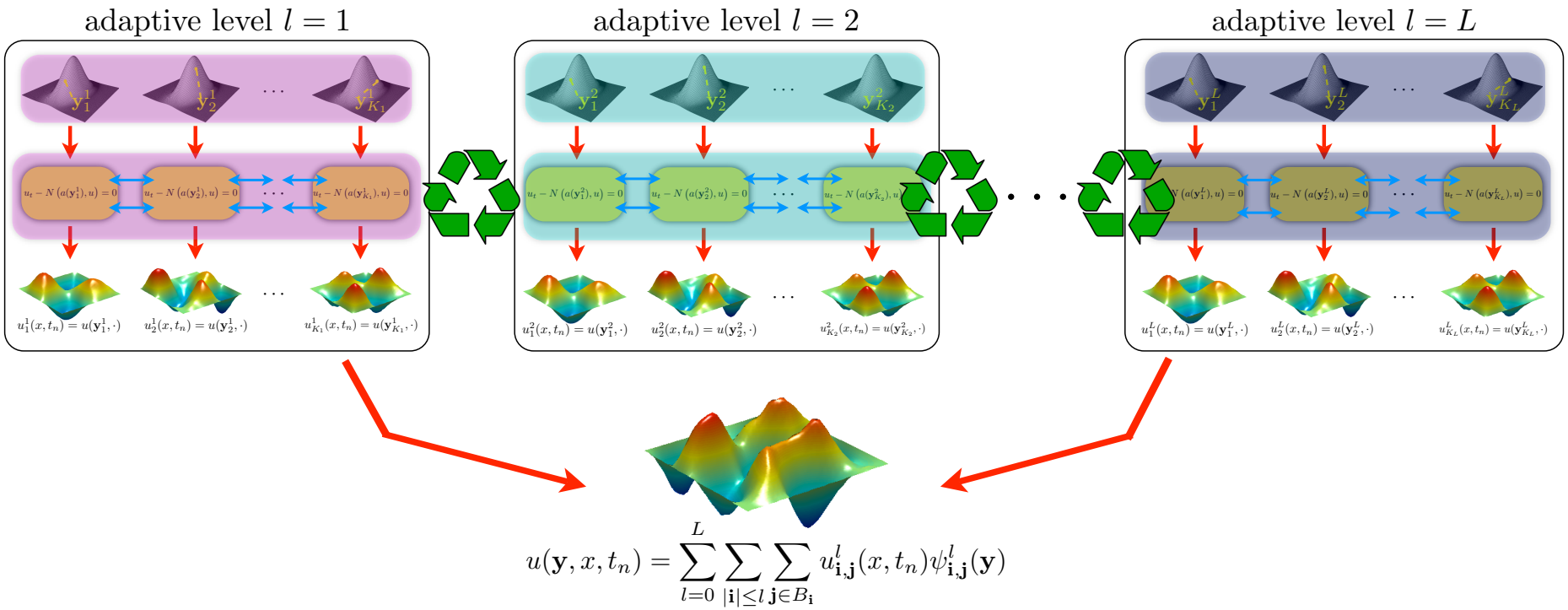
Multilevel hierarchical UQ methods

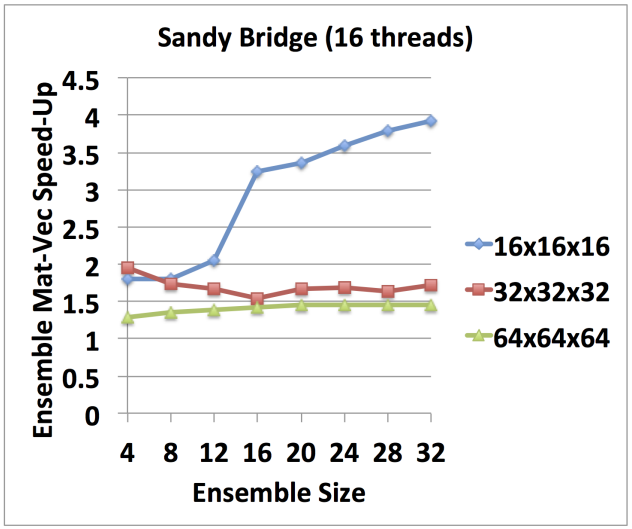
Reduce, reuse and recycle - exploit the hierarchies!

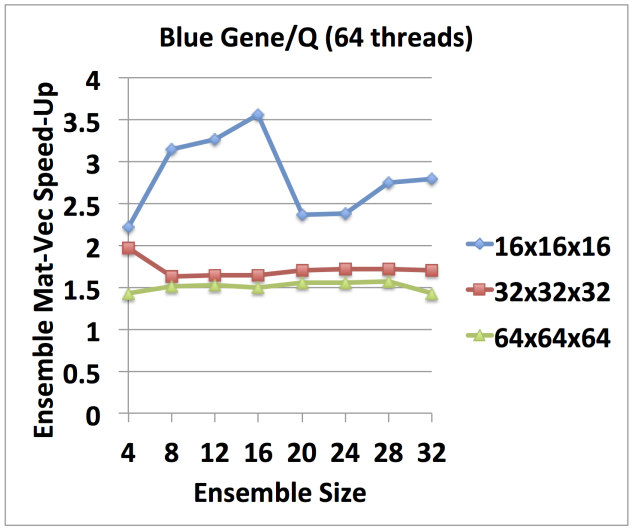


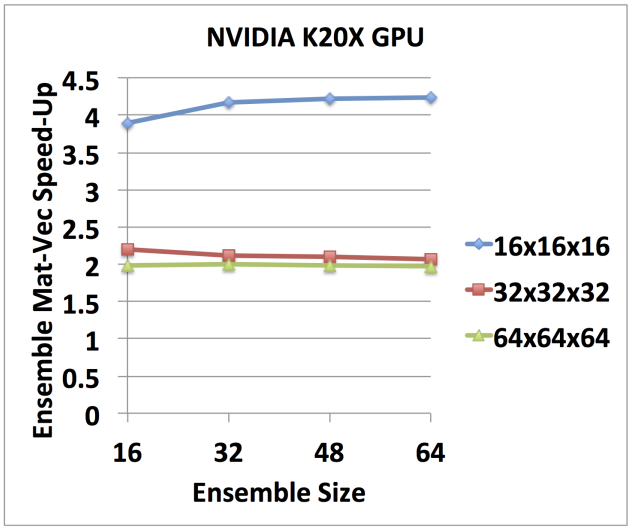
- Exploit similarities between block system across the hierarchical adaptive levels of both the deterministic and stochastic approximations
- *Embedded UQ* approach permits recycling Krylov subspace solvers, providing another opportunity to reduce time-to-solution and memory consumption through reduced solver iterations

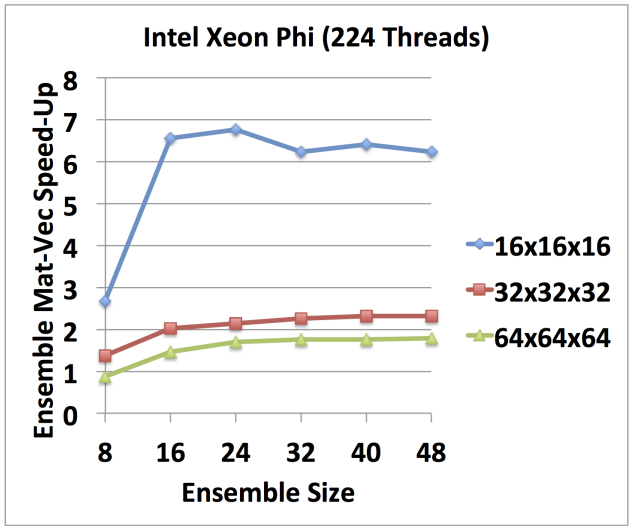
Embedded UQ methods

Ensemble AMG-preconditioned CG speed-up



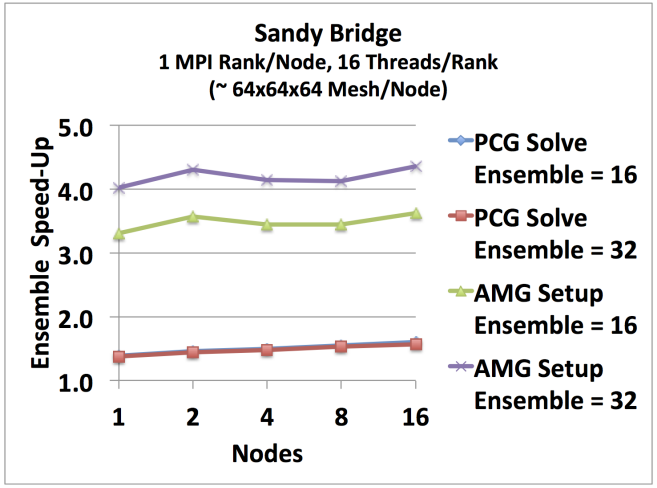


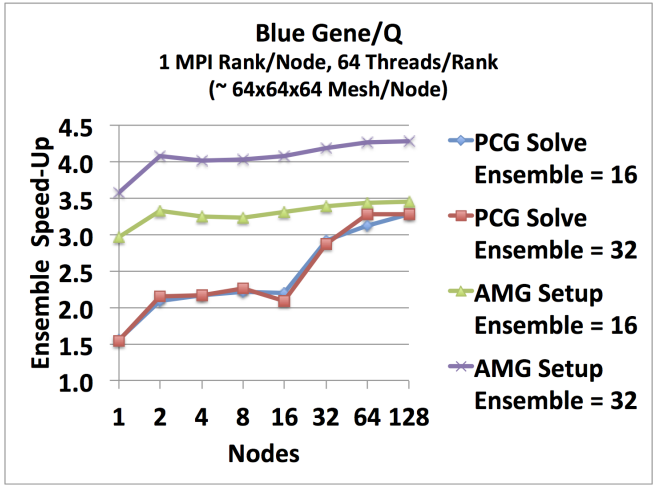


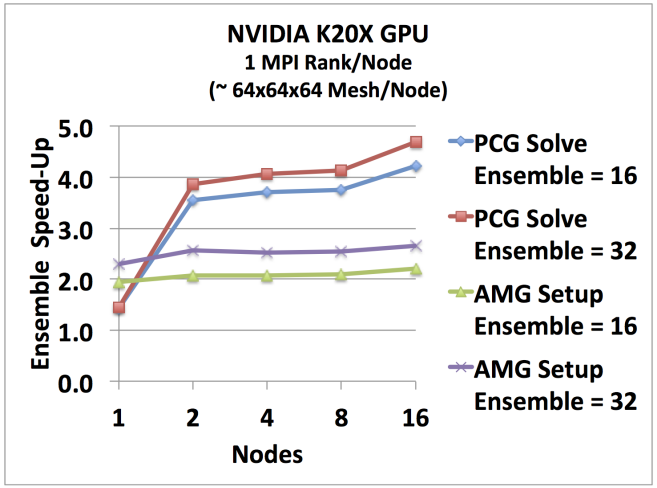


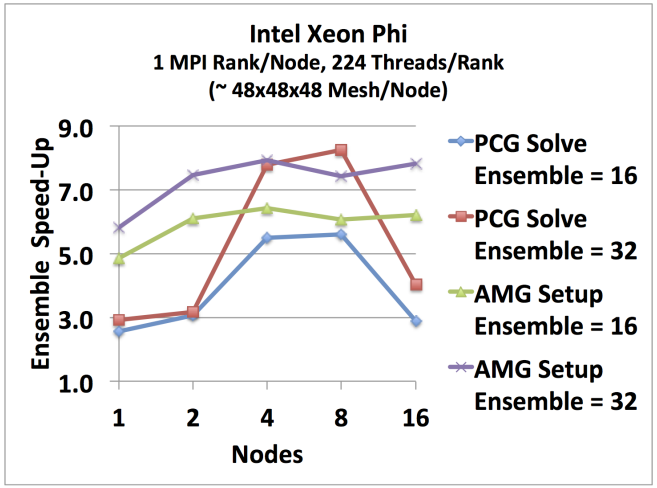
Embedded UQ methods

Ensemble matrix-vector product speed-up









Hierarchical stochastic collocation (HSC) methods

Complexity reduction through solution acceleration

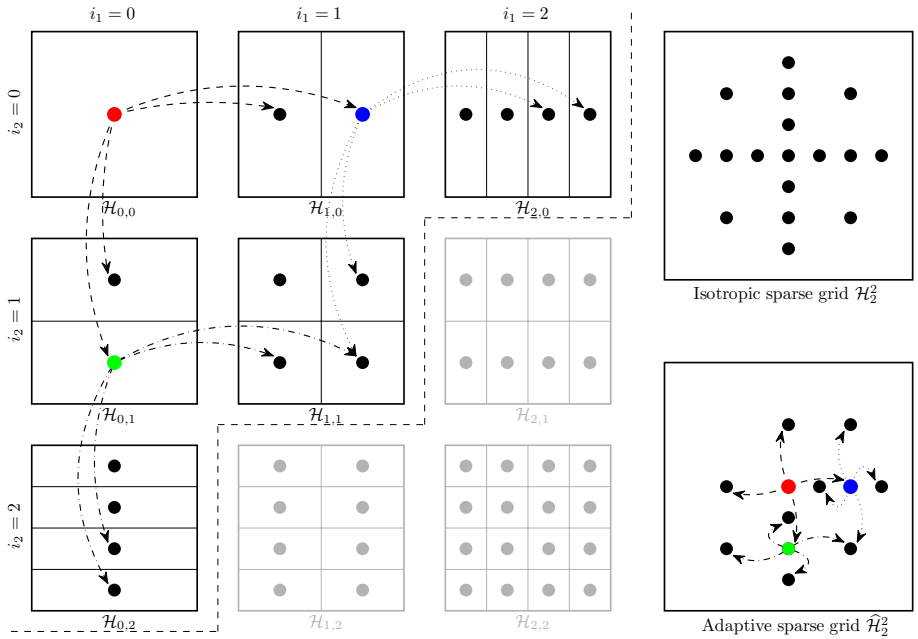
At level $L \in \mathbb{N}_+$, a hierarchical SC approximation is (informally) defined by:

$$u_{M_L,h} = \mathcal{I}_{M_L}[u_h] \equiv \mathcal{I}_{M_{L-1}}[u_h] + \Delta_L[u_h]$$

- $\mathcal{I}_{M_{L-1}}[u_h]$ is the hierarchical interpolant at level $L-1$, and $\Delta_L[u_h]$ is the corresponding hierarchical surplus interpolant at level L

An approach for reducing complexity - exploit the stochastic hierarchy

Construct lower level interpolants $u_{M_{L-1},h}(x, \widetilde{\boldsymbol{y}}_k)$ for $\{\widetilde{\boldsymbol{y}}_k\} \in \Delta\mathcal{H}_{M_L}$ as an initial guess for $u_{M_L,h}(x, \boldsymbol{y})$, to accelerate the underlying (iterative) deterministic solvers

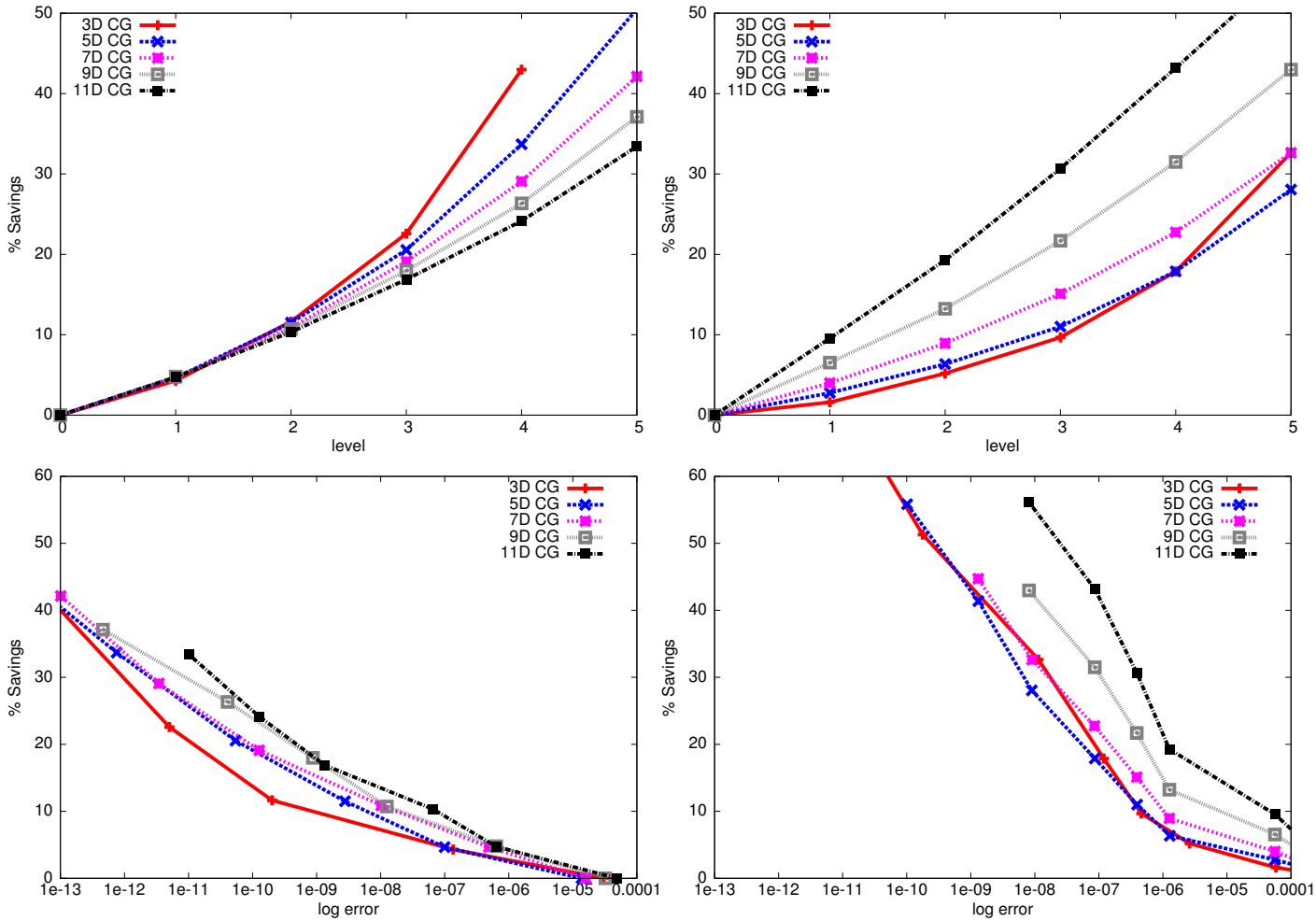


[Gunzburger-W-Zhang, 2013, Jantsch-Galindo-W-Zhang, 2014]

Computational savings of HSC methods

QoI $= \mathbb{E}[u]$ for nonlinear elliptic SPDEs (CG iterative solver)

Figure Savings versus level and savings versus error for $L = 1/64$ (left) and $L = 1/2$ (right)

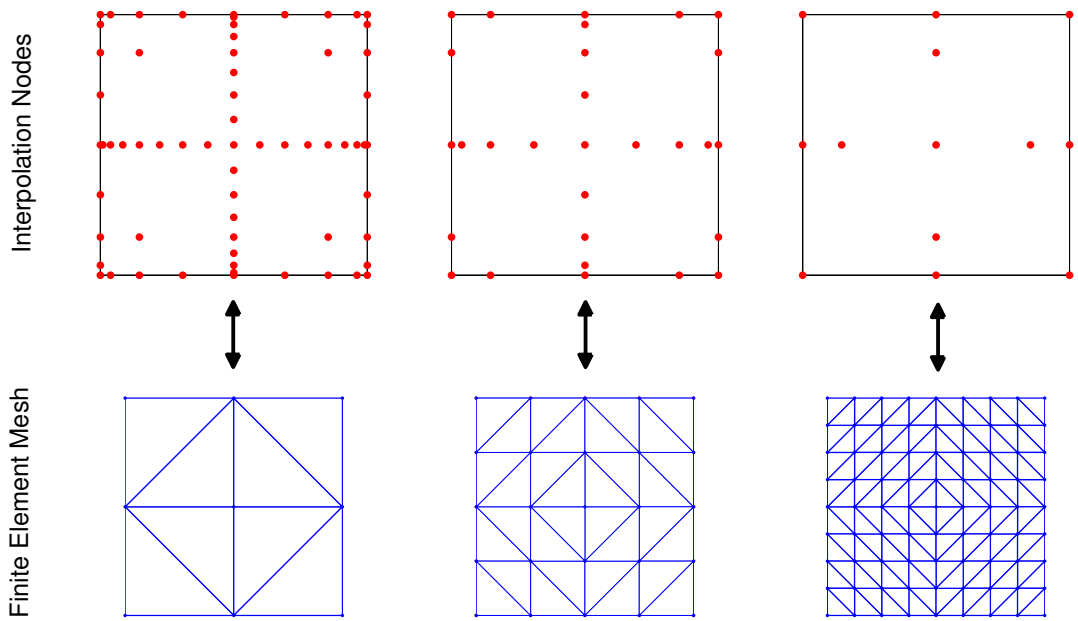


Multilevel stochastic collocation (MLSC) methods

Exploit the deterministic hierarchy [Gunzburger-Jantsch-Teckentrup-W, 2014]

Basic idea: As in the single level case, to increase convergence (compared to MLMC), we simply interpolate the differences $u_{h_k} - u_{h_{k-1}}$ at different resolutions

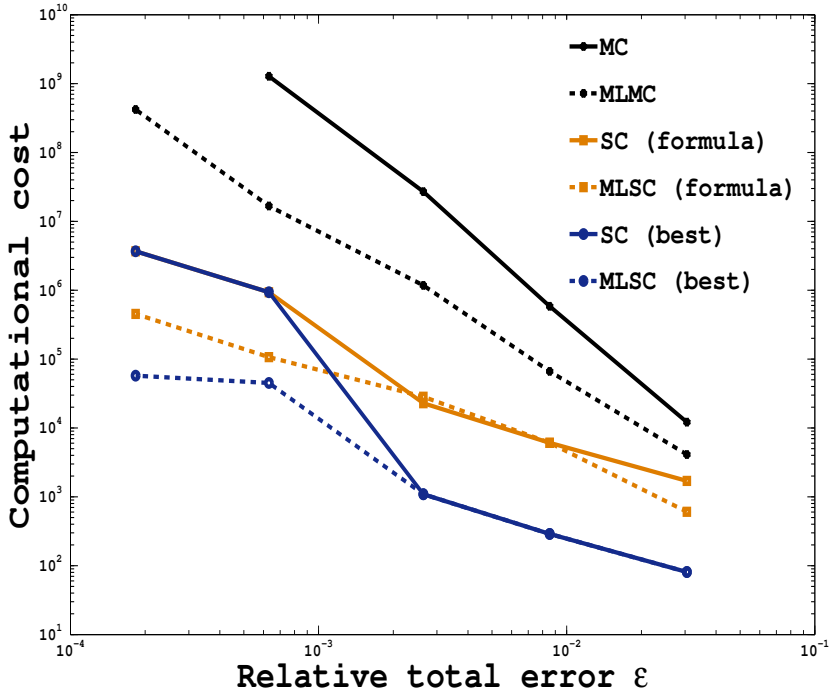
$$u_K^{(MLSC)} = \sum_{k=0}^{K} \mathcal{I}_{M_{K-k}} \left[u_{h_k} - u_{h_{k-1}} \right] = \sum_{k=0}^{K} \left(u^{(\mathrm{SL})}_{M_{K-k},h_k} - u^{(\mathrm{SL})}_{M_{K-k},h_{k-1}} \right)$$



- For a given accuracy, multilevel methods seek to reduce complexity by spreading computational cost evenly across several resolutions of the spatial discretization

Computational savings of MLSC methods

Results in 10D



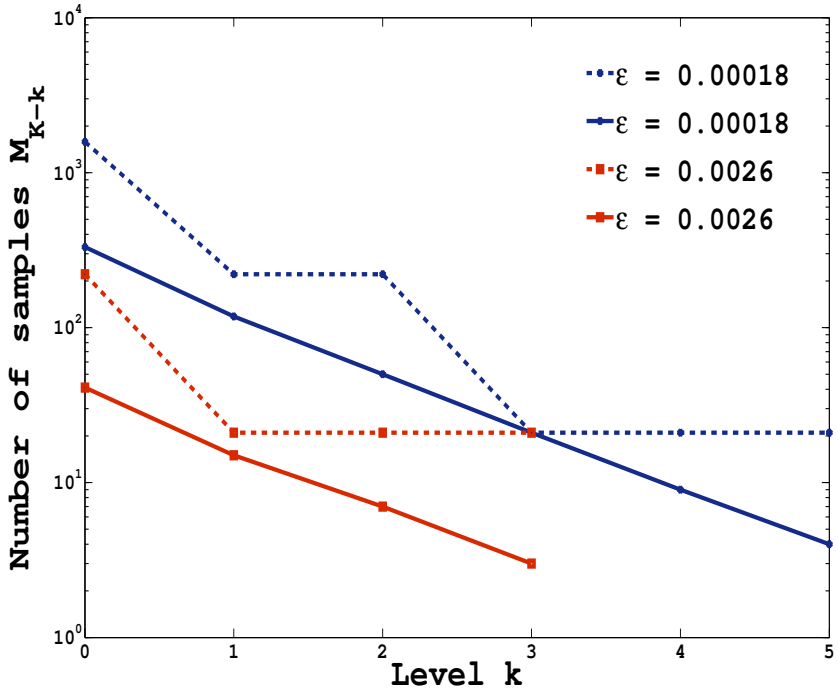
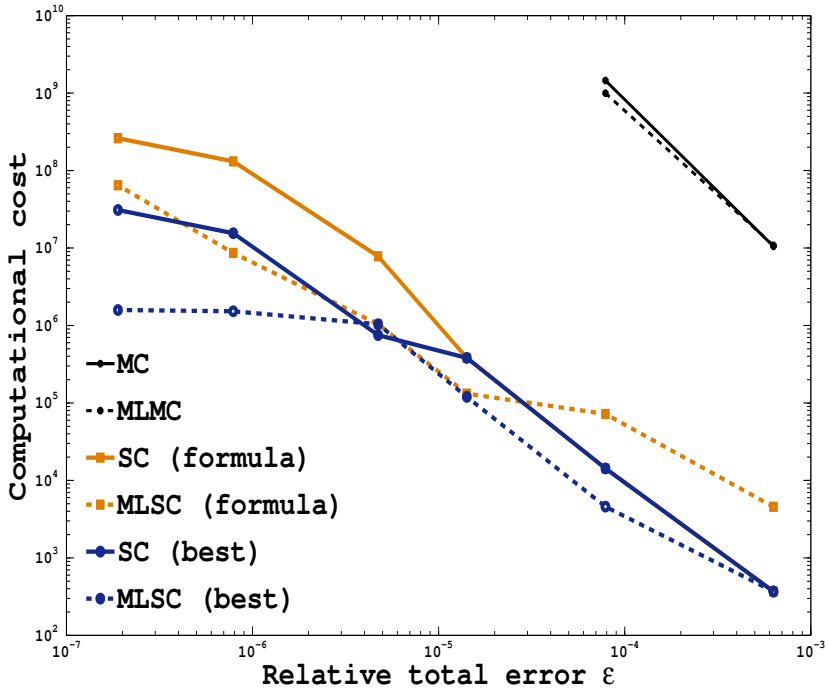


Figure Left: Cost versus Error for $D = (0, 1)^2$, $N = 10$. Right: Number of samples per level (predicted vs actual).

Computational savings of MLSC methods

Results in 20D



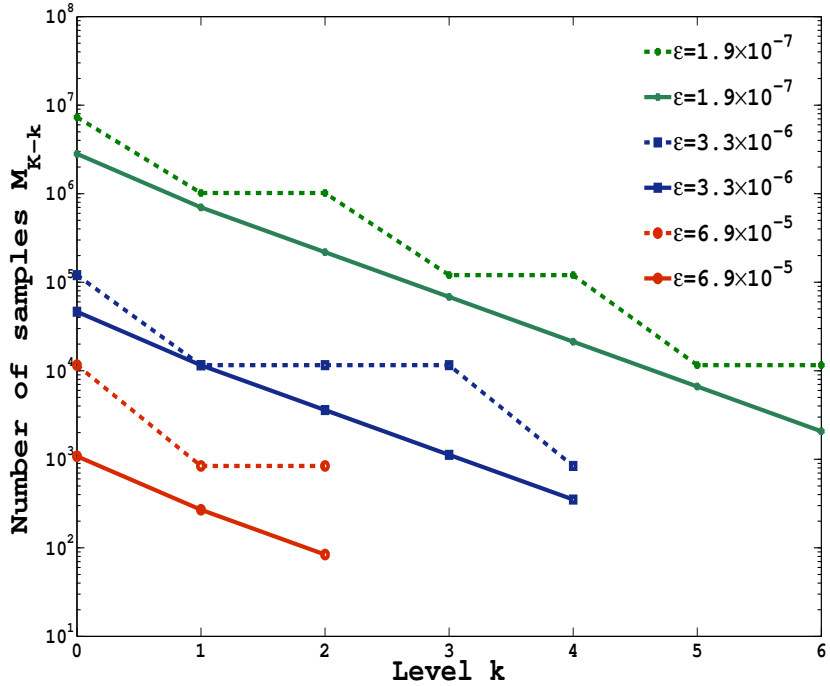


Figure Left: Cost versus Error for $D = (0, 1)$, $N = 20$. Right: Number of samples per level (predicted vs actual).

Optimization and Exascale Computing

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Expect exascale computing to:

- Enable consideration of optimal design for new application areas
- Drive new (at this scale/difficulty level) optimization problems
  - Mixed-integer PDE-constrained optimization
  - Global optimization
  - Robust optimization, Optimization under uncertainty
- Require fundamentally different algorithmic approaches
  - Breaking outer optimization loop-inner simulation separation
  - Concurrent/multi-point function-derivative-subproblem evaluations
  - Multifidelity/hierarchical methods
  - Algorithm-based fault tolerance

New Paradigms

Mixed-Integer PDE-Constrained Optimization Under Uncertainty

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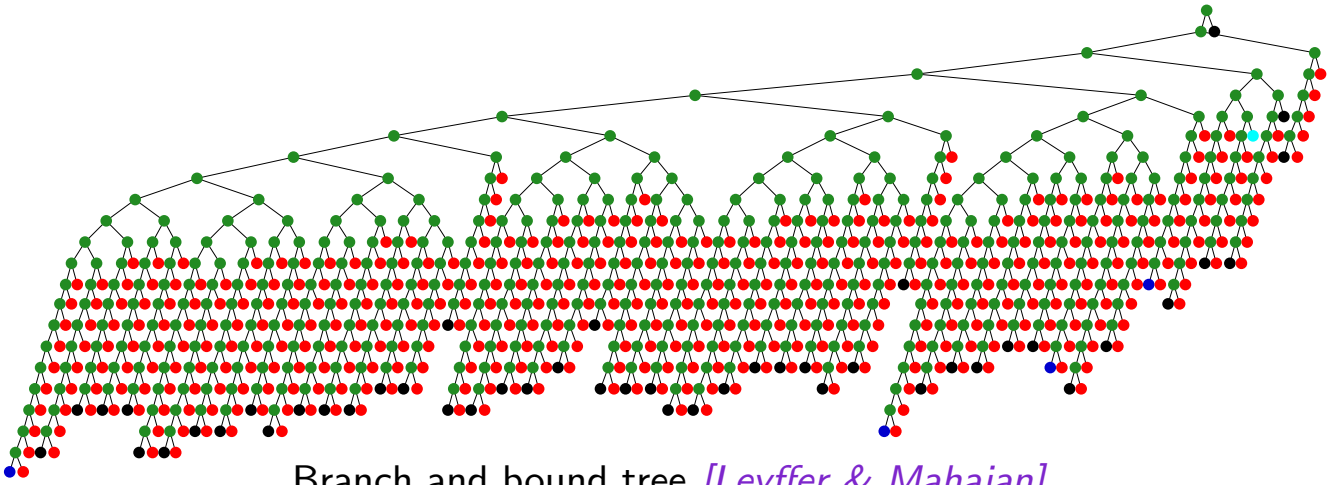
$$\min_{\mathbf{x},\boldsymbol{y}(\omega),\mathbf{z}} \{\mathbb{E}_\omega \left[f(\mathbf{x};\boldsymbol{y}(\omega);\mathbf{z})\right] : \mathbf{c}(\mathbf{x};\boldsymbol{y}(\omega);\mathbf{z};\omega) = 0 \quad \text{a.s. in } \Gamma,\ \forall \mathbf{x} \in \mathcal{X},\ \mathbf{z} \in \mathbb{Z}_z^n \cap \mathcal{Z}\}$$

- $\mathbb{E}f$ Objective
- $\mathbf{x}$ Continuous design variables
- $\boldsymbol{y}(\omega)$ State variables depending on random variables $\omega \in \Omega$
- $\mathbf{z}$ Integer design variables
- $\mathbf{c}$ Linking constraints (PDE and boundary conditions)
- $\mathcal{X}, \mathcal{Z}$ Design constraints

New Paradigms

Sample Challenges/Opportunities

MIPDECO adds a combinatorial explosion to PDECO



Branch and bound tree *[Leyffer & Mahajan]*

- Each node is a PDECO solve
- Rethink today's PDECO (e.g., *[Biros & Ghattas: LNKS]*)
  - Integrate multilevel combinatorial with multilevel PDE
  - Map related PDE/PDECO solves to machine to exploit reuse
  - Allow for approximate/multifidelity PDE/PDECO solves

Mathematical/Numerical Optimization

Today's Generic Methods

Current iterate $\mathbf{x}^k \in \mathbb{R}^n$

1. Generate direction(s) $\mathbf{d}^k \in \mathbb{R}^n$
   - Ex- Newton(-Krylov) direction: $\mathbf{H}^k\mathbf{d}^k = (\approx) -\mathbf{g}^k$
     $\mathbf{H}^k \approx \nabla^2 f(\mathbf{x}^k)$ (or $\nabla^2 L(\mathbf{x}^k)$),
     $\mathbf{g}^k \approx \nabla f(\mathbf{x}^k)$ (or $\nabla L(\mathbf{x}^k)$)
   - Ex- Sequential quadratic programming:
     $\min_{\mathbf{d}\in\mathbb{R}^n} \left\{\mathbf{d}^T\mathbf{H}^k\mathbf{d} + \mathbf{d}^T\mathbf{g}^k : \nabla\mathbf{c}(\mathbf{x}^k)\mathbf{d} + \mathbf{c}(\mathbf{x}^k) = 0\right\}$
   - Ex- Stochastic: $-\left(\nabla f(\mathbf{x}^k)^T\mathbf{d}^k\right)\mathbf{d}^k$, random $\mathbf{d}^k$
2. Determine step length $\alpha^k > 0$
   - Ex- Line search: approximately solve
     $\min_{\alpha\geq 0} \phi(\mathbf{x}^k + \alpha\mathbf{d}^k)$ using merit function ϕ
   - Ex- Trust region: constrain $\|\alpha^k\mathbf{d}^k\| \leq \Delta^k$
   - Ex- Fixed step size: $\alpha_k = \kappa_k$
3. Update $\mathbf{x}^{k+1} = \mathbf{x}^k + \alpha^k\mathbf{d}^k$,
   evaluate $f(\mathbf{x}^{k+1})$, $\nabla f(\mathbf{x}^{k+1})$, ...

Inherently sequential iterations

- Typical focus: reduce work/time per iteration
- Appeal to Newton/Nesterov for fast convergence
- Evaluations of f, ∇f, $\mathbf{Hv}$, ... occur sequentially
- Requires global synchronization at each k (except for very special cases)

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Today's Parallel Methods

Single Point per Iteration

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1. Parallelize linear algebra within iteration
   - Used to evaluate f, ∇f, ...
   - Matrix-free Jacobian-/Hessian-vector products

     Ex.- Toolkit for Advanced Optimization based on PETSc *[Munson et al]*

   Exa! Explosion of concurrency: optimization must take part

2. Multilevel optimization methods
   - Rely primarily on grid structure for variables

     Ex- *[Toint et al]*, *[MG/OPT: Lewis & Nash]*

   Exa! Does not fully account for architectural hierarchies, adaptivity, multiphysics, ...

3. Assume function (+derivative) evals succeed at demanded tolerance

   Exa! Pay price for demanding resilient computation

   Exa! Analysis for ABFT to enlarge classes of failures under which some form of convergence still ensured

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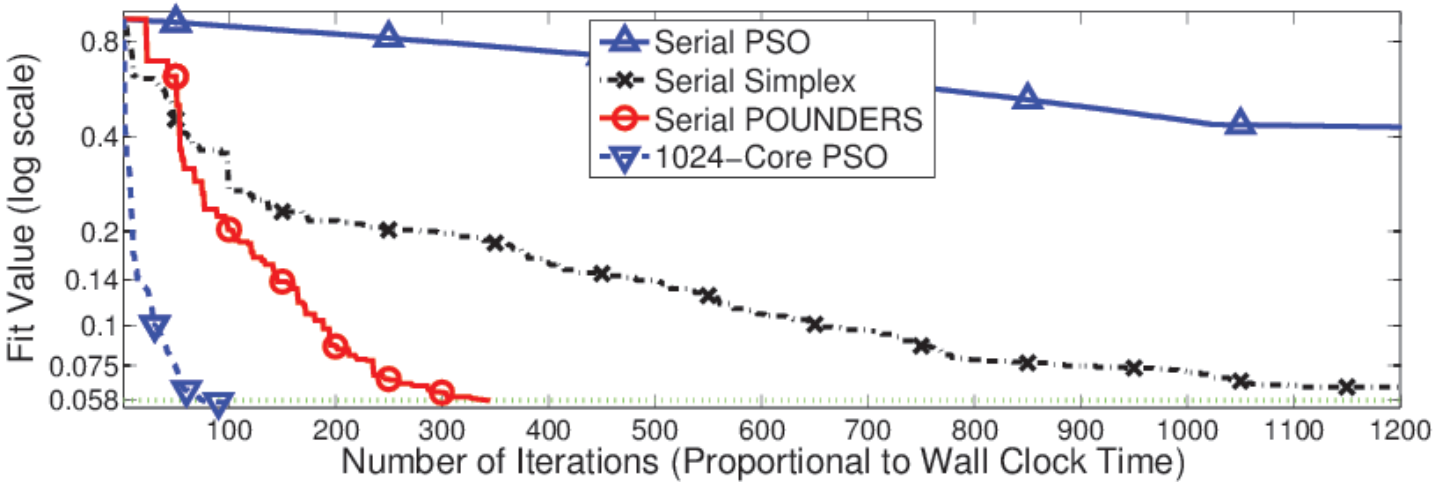
Today's Parallel Methods

Concurrent Evaluations

- Primarily for derivative-free methods (e.g., $\nabla f(\mathbf{x})$ unavailable)
  - Ex- `HOPSPACK` *[Kolda et al]*: Evaluate $\{f(\mathbf{x}^k + \mathbf{d}_i) : i = 1, \ldots, p\}$ concurrently
  - Ex- `VTDIRECT` *[Watson et al]*: Concurrent evals for (approx) global optimization
  - Ex- `POUNDERS` *[W.]*: Evaluate residuals concurrently
  - Ex- Heuristics (GAs, particle swarm, ...): Concurrent generation evaluation

- Poor scaling of time to solution with respect to # of concurrent evals



  - Ex- `POUNDERS` (single evaluation) only 3 times slower than PSO (1024 concurrent evals) on accelerator design problem

Require New Methods and Analysis

Increased Concurrency for Derivative-Based Solvers?

Analysis to determine classes of problems where this works

- Krylov-based solutions to $\min_{\mathbf{x}\in\mathbb{R}^n}\{\|\mathbf{Ax}-\mathbf{b}\|\}$
  - s-step methods *[Chronopoulos 1991]*
  - CA/CH methods using matrix power kernel $\mathbf{Au}, \mathbf{A}^2\mathbf{u}, \ldots$
- Increase arithmetic intensity by evaluating local ensembles of related points
- Subspace/decomposition techniques
  - Trivial for separable problems ($\mathbf{x}_i \cap \mathbf{x}_j = \emptyset, i \neq j$):

$$\min_{\mathbf{x}\in\mathbb{R}^n}\left\{\sum_{i=1}^{p} f_i(\mathbf{x}_i)\right\} \quad \longrightarrow \quad \min_{\mathbf{x}_i\in\mathbb{R}^{n_i}}\left\{f_i(\mathbf{x}_i)\right\},\ i=1,\ldots,p$$

  - More general: orthogonal/iterated subspaces + a synchronization step *[Gould et al, 1994]*, *[Yuan, 2007]*, *[Gratton et al, 2014]*

Decomposition to Reduce Outer Iterations

Back to the Future

Parallel variable distribution *[Ferris & Mangasarian, 1994]*

1. Generate partitioned direction $\mathbf{d} = (\mathbf{d}_1, \ldots, \mathbf{d}_p) \in \mathbb{R}^n$, $\mathbf{d}_i \in \mathbb{R}^{n_i}$
   - Not block Jacobi/coordinate search because of $\mathbf{d}$
   - $\mathbf{d}$: Newton direction, steepest descent, ...
2. Concurrently solve p $(n_i + p - 1)$-dimensional subproblems

$$\min_{\mathbf{x}_i \in \mathbb{R}^{n_i}, \mathbf{u}_i \in \mathbb{R}^{p-1}} \{f(\mathbf{x}_i, \mathbf{D}_{-i}\mathbf{u}_i) : (\mathbf{x}_i, \mathbf{D}_{-i}\mathbf{u}_i) \in \mathcal{X}\}$$

   to obtain $\boldsymbol{y}^i = (\mathbf{x}_i, \mathbf{D}_{-i}\mathbf{u}_i) \in \mathbb{R}^n$

3. Obtain $\mathbf{x}^{k+1} = v_{p+1}\mathbf{x}^k + \sum_i v_i \boldsymbol{y}^i$ from $(p+1)$-dimensional subproblem

$$\min_{\mathbf{v} \in \mathbb{R}^{p+1}} \left\{ f\left(v_{p+1}\mathbf{x}^k + \sum_i v_i \boldsymbol{y}^i \right) : v_{p+1}\mathbf{x}^k + \sum_i v_i \boldsymbol{y}^i \in \mathcal{X}, \quad \mathbf{v}^T\mathbf{e} = 1 \right\}$$

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Parallel variable distribution *[Ferris & Mangasarian, 1994]*

1. Generate partitioned direction $\mathbf{d} = (\mathbf{d}_1, \ldots, \mathbf{d}_p) \in \mathbb{R}^n$, $\mathbf{d}_i \in \mathbb{R}^{n_i}$
   - Not block Jacobi/coordinate search because of $\mathbf{d}$
   - $\mathbf{d}$: Newton direction, steepest descent, ...
2. Concurrently solve p $(n_i + p - 1)$-dimensional subproblems

$$\min_{\mathbf{x}_i \in \mathbb{R}^{n_i}, \mathbf{u}_i \in \mathbb{R}^{p-1}} \{f(\mathbf{x}_i, \mathbf{D}_{-i}\mathbf{u}_i) : (\mathbf{x}_i, \mathbf{D}_{-i}\mathbf{u}_i) \in \mathcal{X}\}$$

   to obtain $\boldsymbol{y}^i = (\mathbf{x}_i, \mathbf{D}_{-i}\mathbf{u}_i) \in \mathbb{R}^n$

3. Obtain $\mathbf{x}^{k+1} = v_{p+1}\mathbf{x}^k + \sum_i v_i \boldsymbol{y}^i$ from $(p+1)$-dimensional subproblem

$$\min_{\mathbf{v} \in \mathbb{R}^{p+1}} \left\{ f\left(v_{p+1}\mathbf{x}^k + \sum_i v_i \boldsymbol{y}^i \right) : v_{p+1}\mathbf{x}^k + \sum_i v_i \boldsymbol{y}^i \in \mathcal{X}, \quad \mathbf{v}^T\mathbf{e} = 1 \right\}$$

Optimization Under Uncertainty

Example: Sample Average Approximation

Approximately solve stochastic program

$$\min_{\mathbf{x}\in\mathcal{X}\subset\mathbb{R}^n} \{\mathbb{E}_\omega [f(\mathbf{x};\omega)] : \mathbf{c}(\mathbf{x};\omega) = 0 \quad \forall\omega \in \Omega\}$$

by solving

$$\min_{\mathbf{x}\in\mathcal{X}} \left\{ \sum_{i=1}^{N} f(\mathbf{x};\omega_i) : \mathbf{c}(\mathbf{x};\omega_i) = 0,\ i = 1,\ldots,N \right\}$$

using the N scenarios $\omega_1, \ldots, \omega_N$

- Constraint/objective evaluation naturally parallelizable in scenarios
- Specific forms of f, $\mathbf{c}$, $\mathcal{X}$ enable scalable linear algebra
- ! Increased scenarios for exascale concurrency rarely (never?) useful
- ! Number of outer iterations (= global reductions) does not decrease as N grows

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Today's Parallel Methods

SAA at the Petascale

A special case: 2-stage programs

- f convex, quadratic
- C linear (equalities) with a recourse term for each scenario

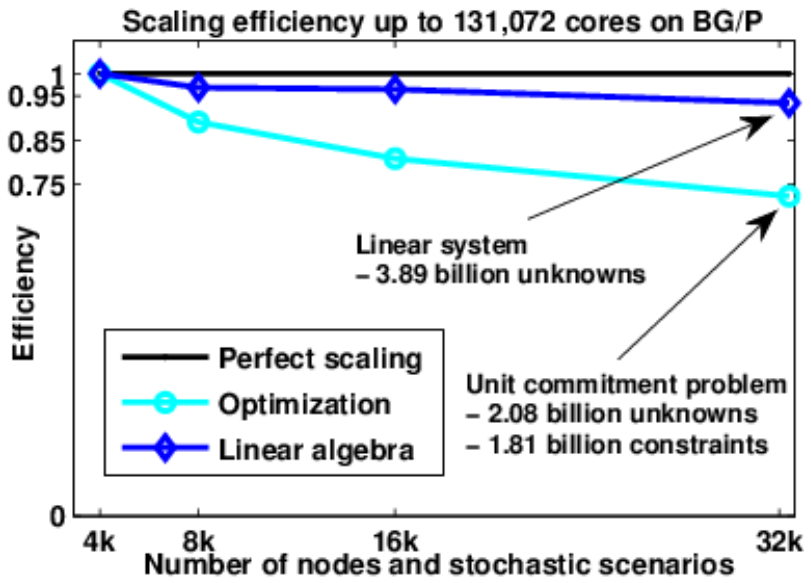
Interior point methods solve arrow systems

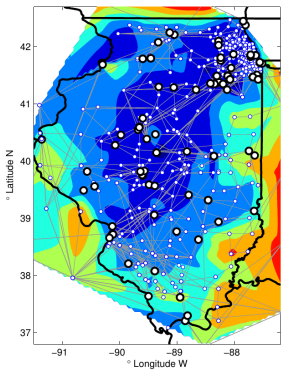
$$\begin{bmatrix} \mathbf{A}_1^k & & & \mathbf{B}_1^k \\ & \ddots & & \vdots \\ & & \mathbf{A}_N^k & \mathbf{B}_N^k \\ \mathbf{B}_1^{k\,T} & \cdots & \mathbf{B}_N^{k\,T} & \mathbf{A}_0^k \end{bmatrix} \delta^{k+1} = \mathbf{r}^k$$

in each iteration.

Dominant expense: Schur complements

$$\mathbf{B}_i^{k\,T} \left(\mathbf{A}_i^k\right)^{-1} \mathbf{B}_i^k$$





Solving energy unit commitment problems using PIPS

[Lubin, Petra, Schenck, Anitescu et al 2011–]

Concluding remarks

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- Exascale optimization and uncertainty quantification methods must break the outer loop mentality:
  - exploitation of shared data structures for reduced memory usage
  - realize massive parallelism through simultaneous propagation
  - solution techniques for selectively coupled systems
  - optimal propagation sets via selective coupling
  - embedded optimization and UQ capabilities will enable confident predictions of new application areas
- Moreover, such embedded approaches will facilitate the acceleration, and thus, reduce overall complexity of (linear and nonlinear) solvers by exploring multilevel methods and exploiting the inherent hierarchies
- Lots of challenges:
  - significant effort to refactor simulation codes
  - solvers/preconditioners must be optimized for embedded approaches
  - memory access patterns will become critical
  - propagating samples together requires commonality in solution process . . .